The extension of Statistical Entropy Analysis to chemical compounds

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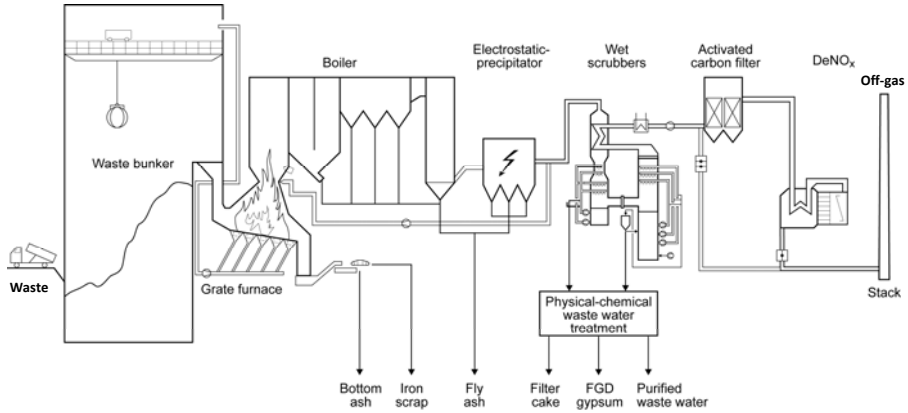
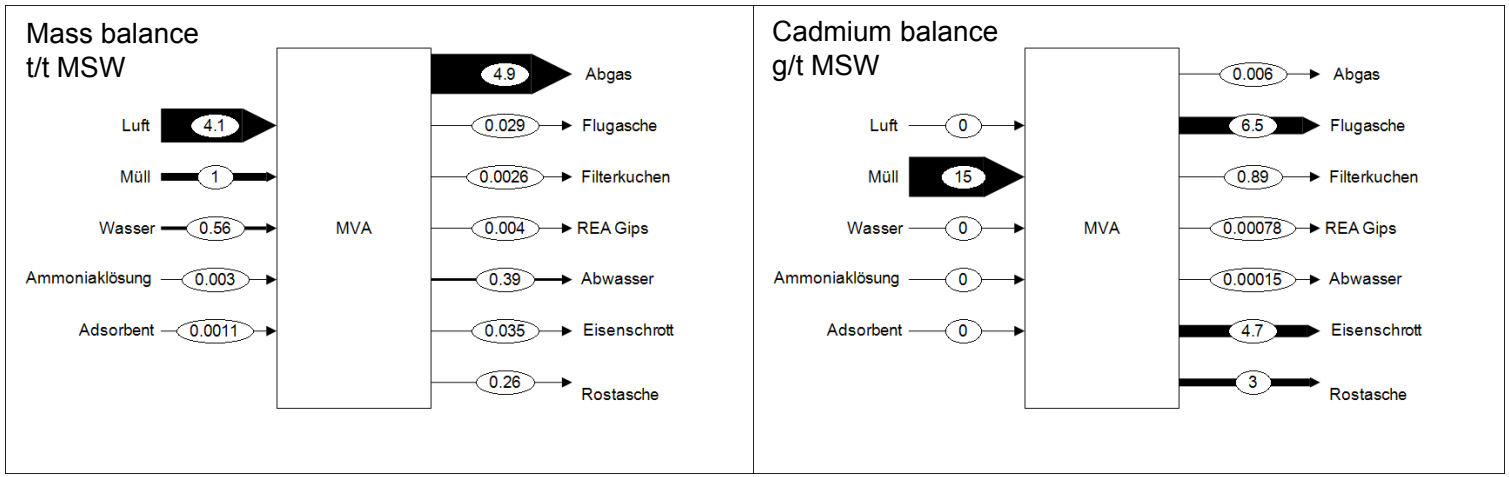
The extension of what….?

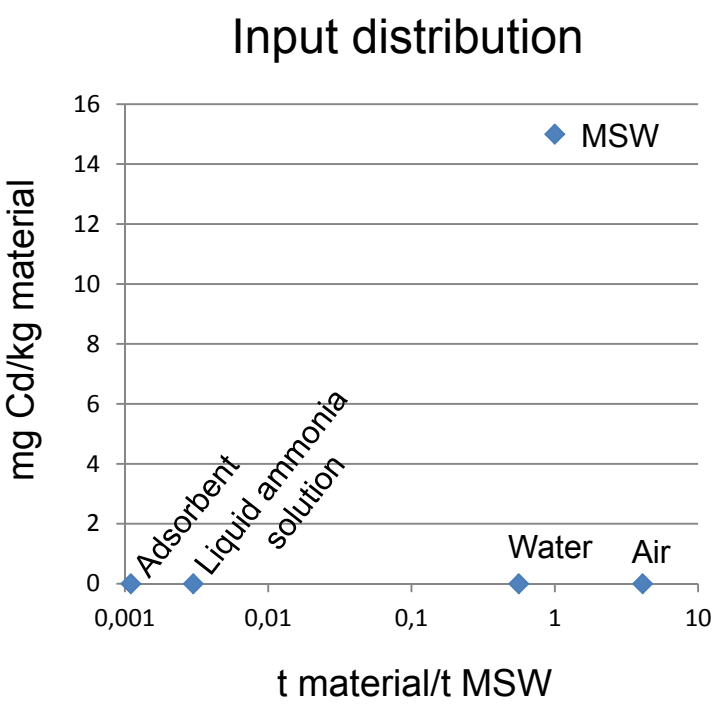
1. Introduction to Statistical Entropy Analysis (SEA)
2. Why is extension required?
3. Applications of extended SEA (eSEA)

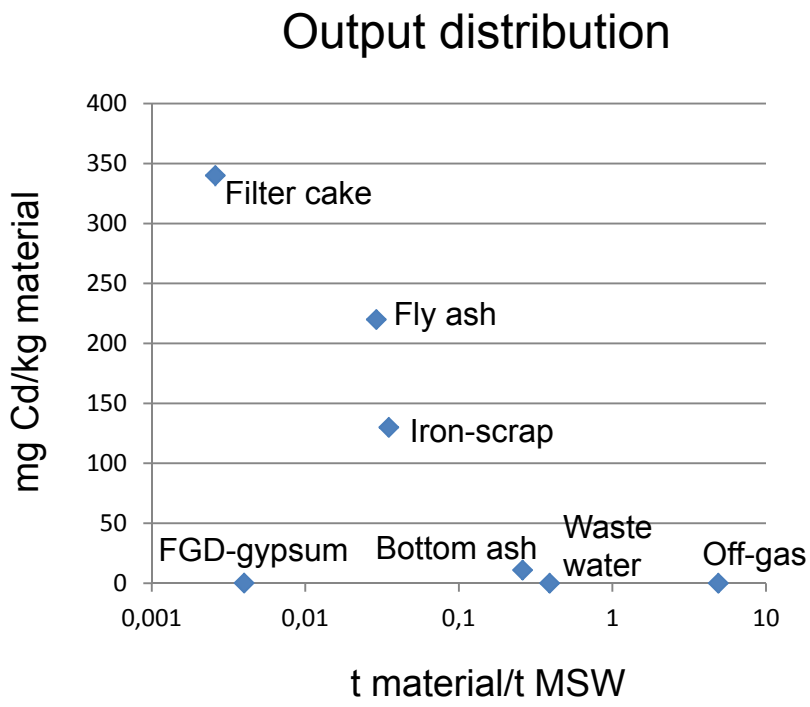
Initial question: concentrating or diluting?



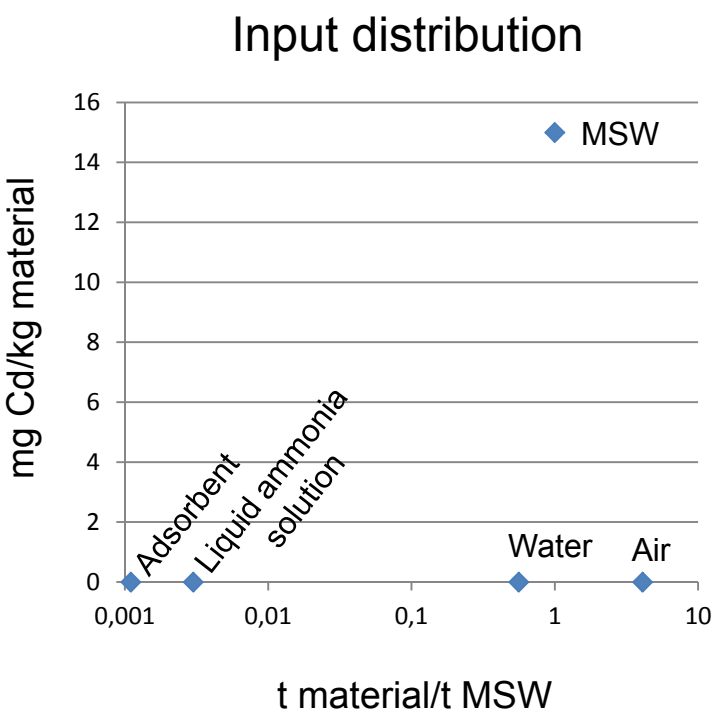


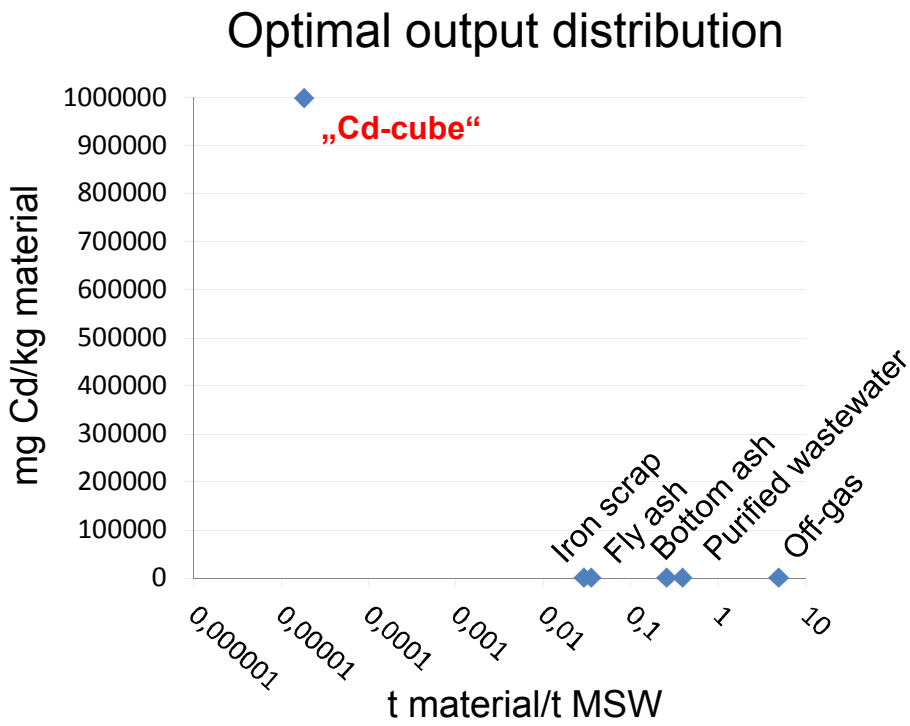
A process changes distributions



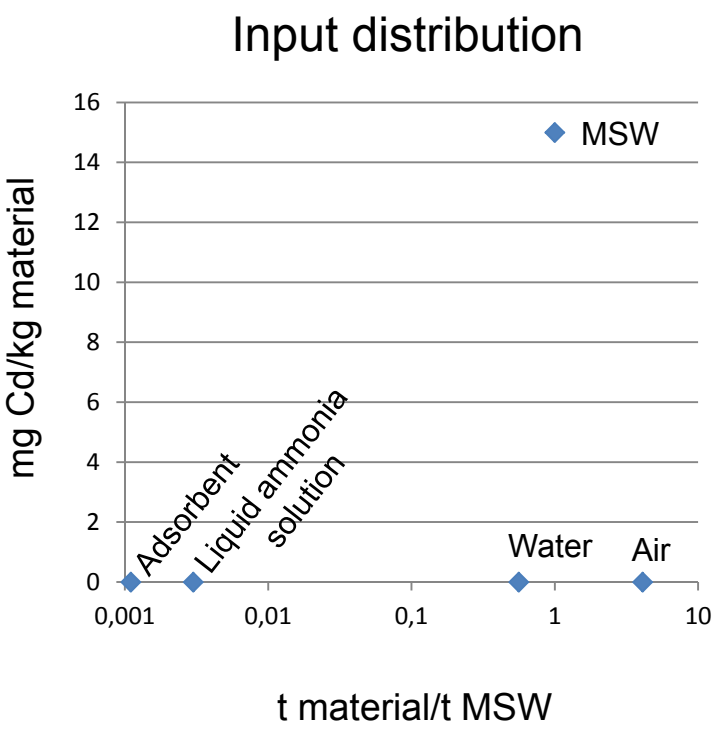


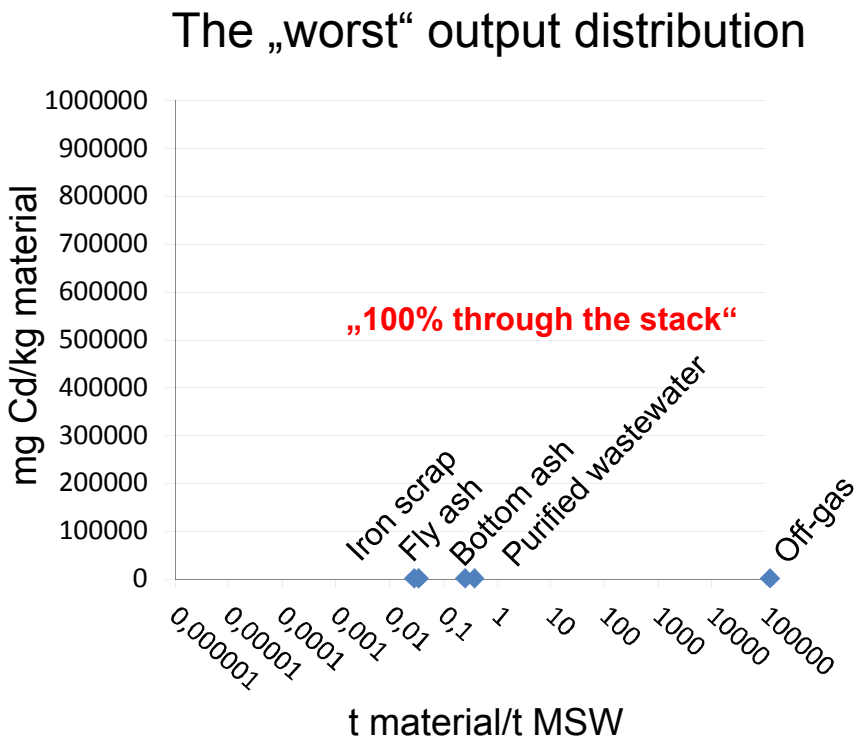
The (hypothetical) optimal process





The (hypothetical) worst process

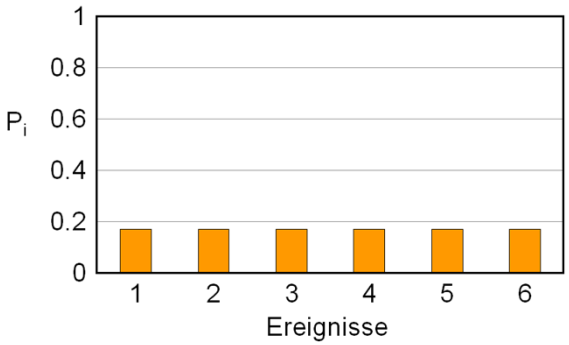




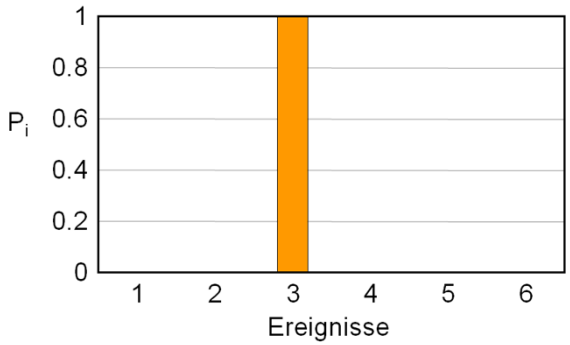
Statistical entropy (SE)

In the science of *descriptive statistics* the entropy is a measure to quantify any distribution.

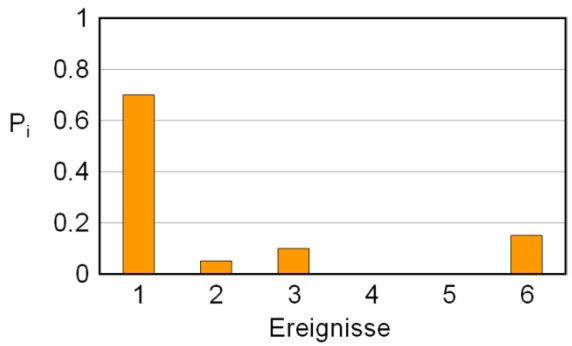
$$H_S = -\sum_{i=1}^{k} P_i \cdot \log_2(P_i) \qquad H_{max} = \log_2(k) \qquad H_{rel} = H_S / H_{max}$$



H_{rel} = 1 = Max

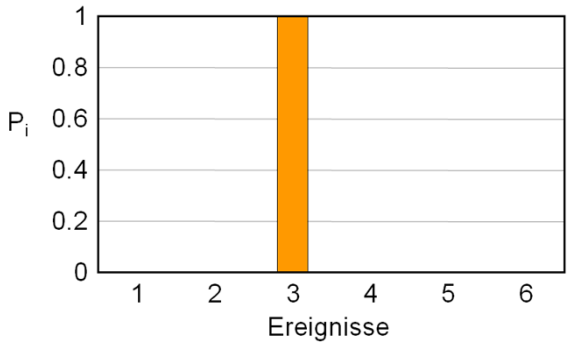


H_{rel} = 0 = Min



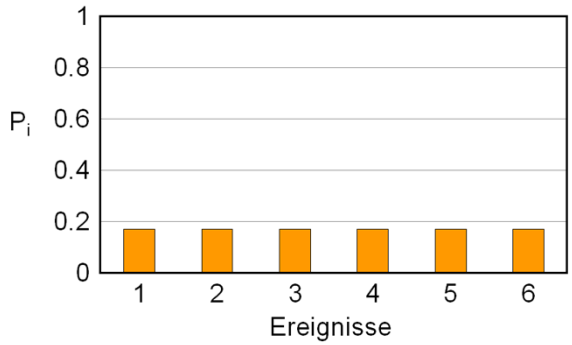
H_{rel} = 0.51

Analogy between playing dice and burning waste



H_{rel} = 0 = Min

„Cd-cube“



H_{rel} = 1 = Max

„100% through the stack“

Making SE applicable to material budgets

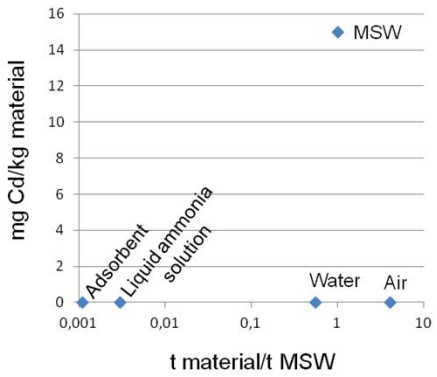
Statistical entropy

$$H_S = -\sum_{i=1}^{k} P_i \cdot \log_2(P_i) \qquad \sum_{i=1}^{k} P_i = 1 \qquad H_{max} = \log_2(k) \qquad H_{rel} = H_S / H_{max}$$

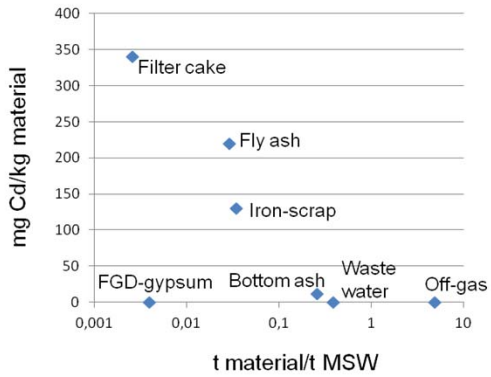
Statistical entropy analysis (Rechberger & Brunner, 2002)

$$H_S = -\sum_{i=1}^{k} m_i \times c_i \times \log_2(c_i) \qquad \sum_{i=1}^{k} c_i \times m_i = 1 \qquad H_{max} = \log_2\left(\sum_{i=1}^{k} m_i\right)$$

Input distribution



Output distribution



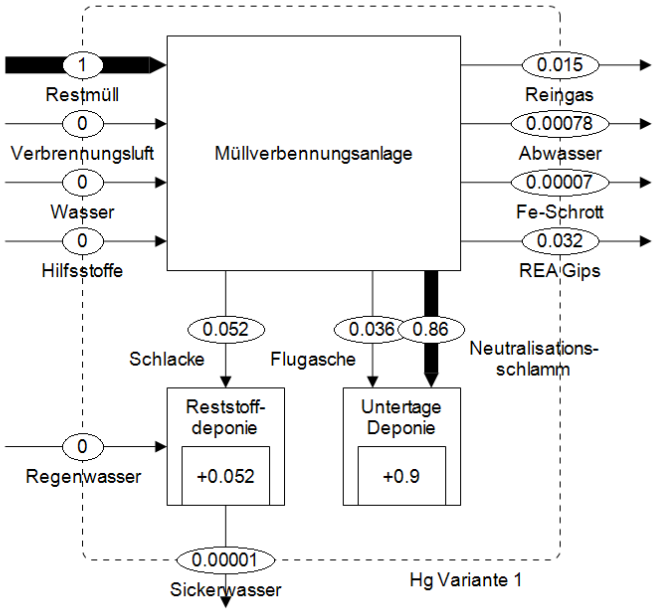
$$\Delta H = H_{OUT} - H_{IN}$$

H_{IN} [0,1]

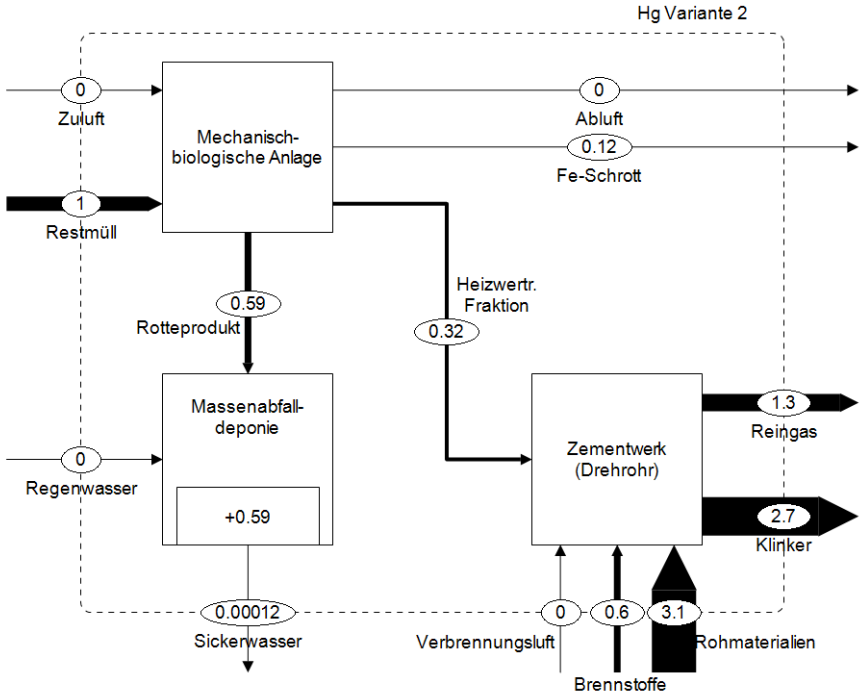
H_{OUT} [0,1]

Hg distributions of two waste management systems

System „Incinerator“



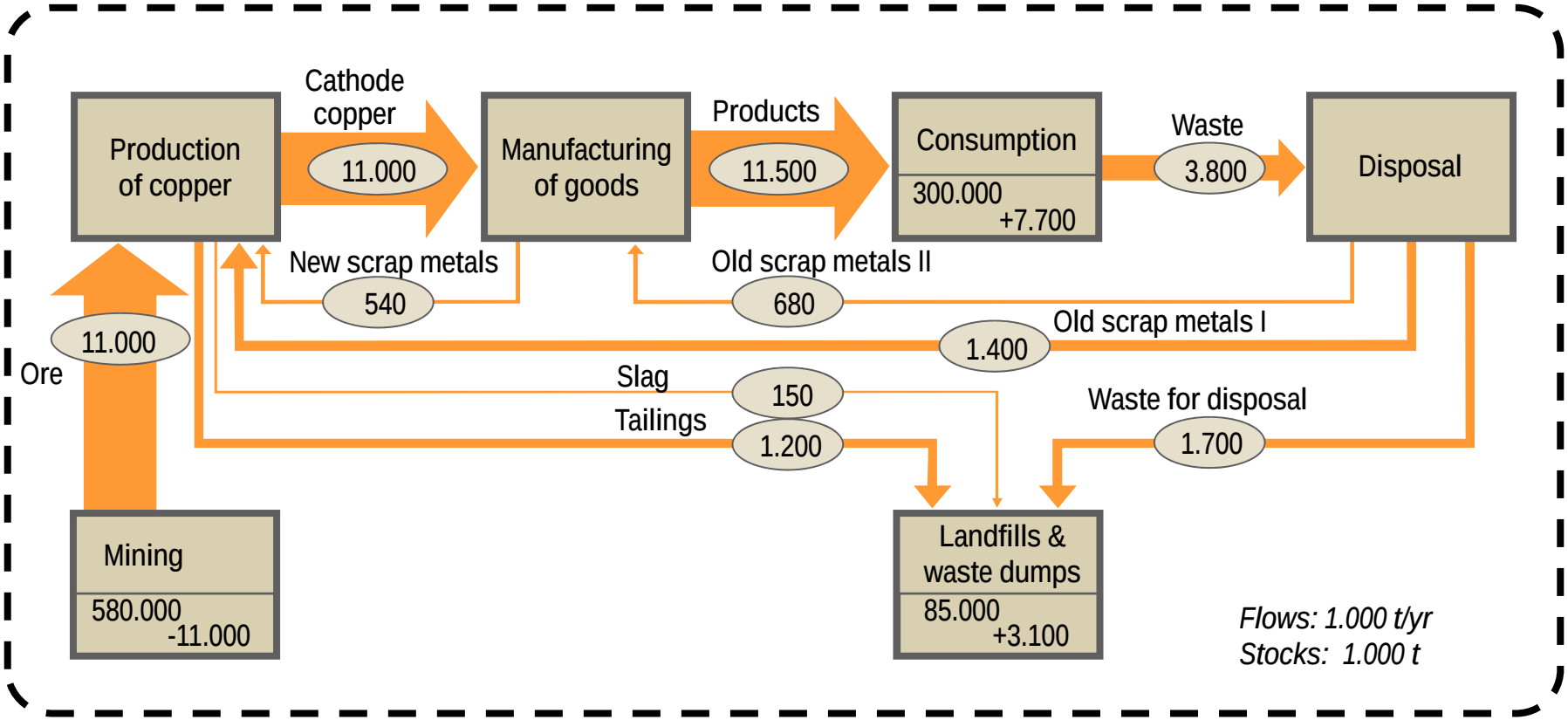
System „MBT + cement kiln“



$H_{IN} = 0.39$
$H_{OUT} = 0.30$
$\Delta H = -23\%$ (= concentrating)

$H_{IN} = 0.39$
$H_{OUT} = 0.46$
$\Delta H = +18\%$ (= diluting)

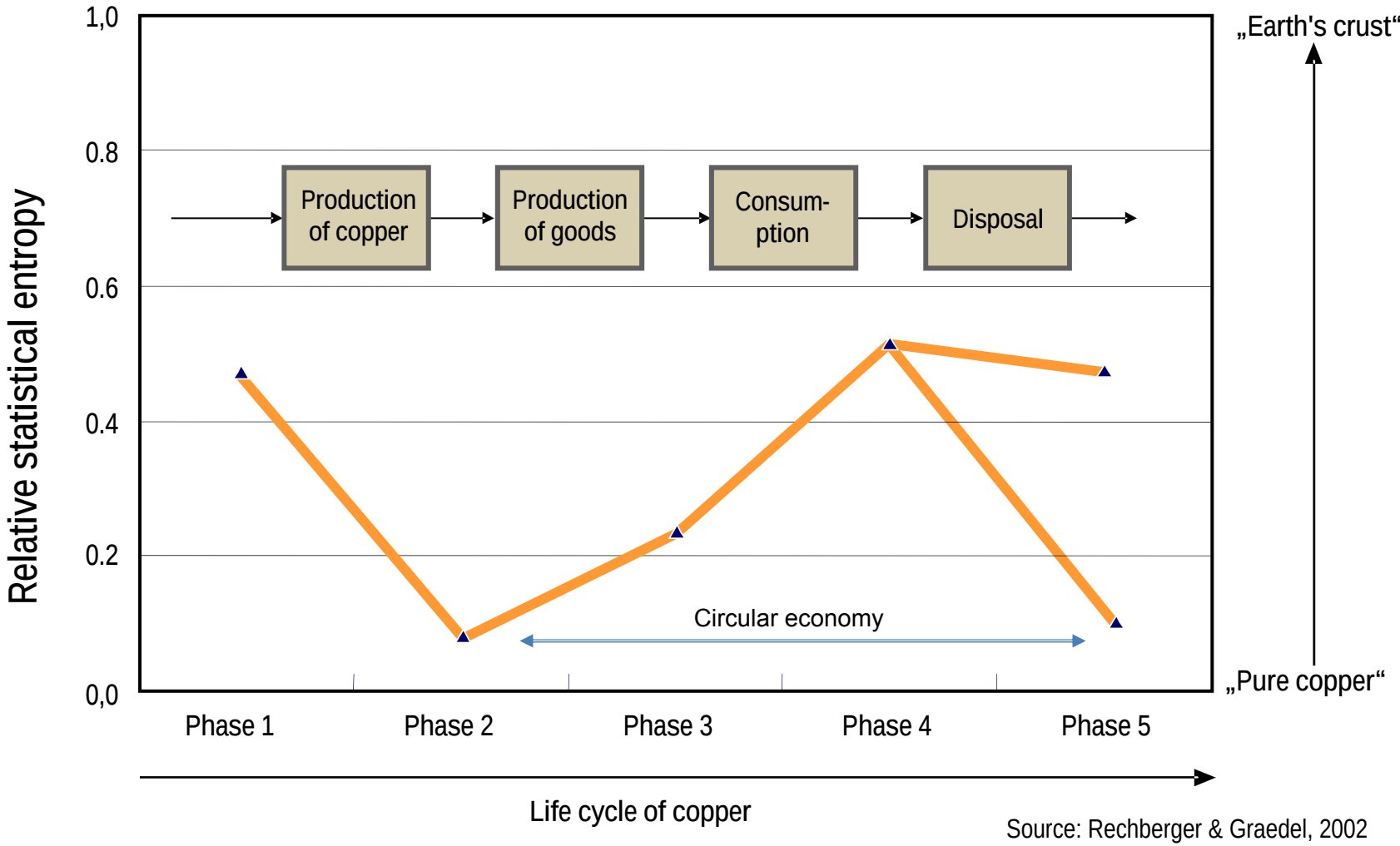
Global copper cycle



System boundary „copper global 1994"

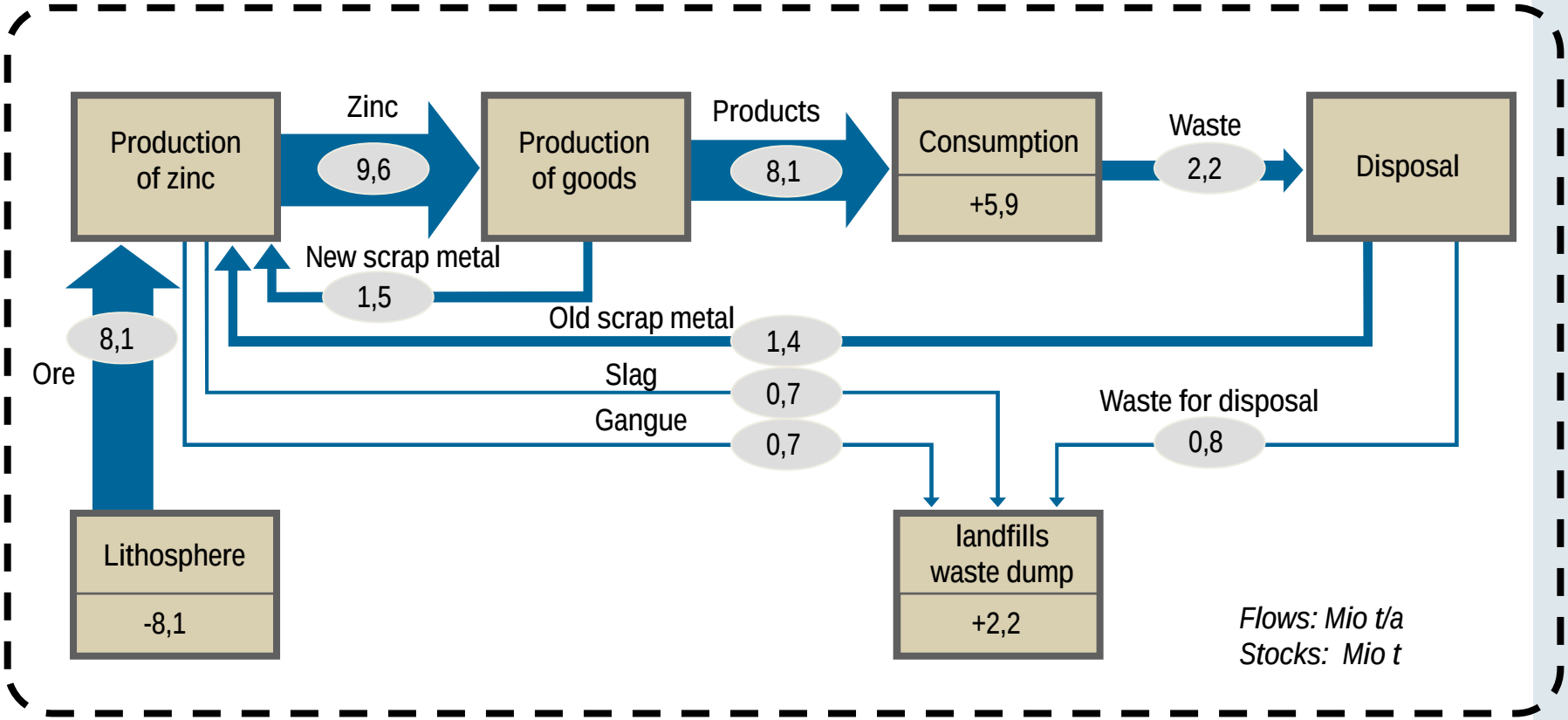
Source: Graedel et al. 2002 (adapted)

Global copper cycle: SEA



Source: Rechberger & Graedel, 2002

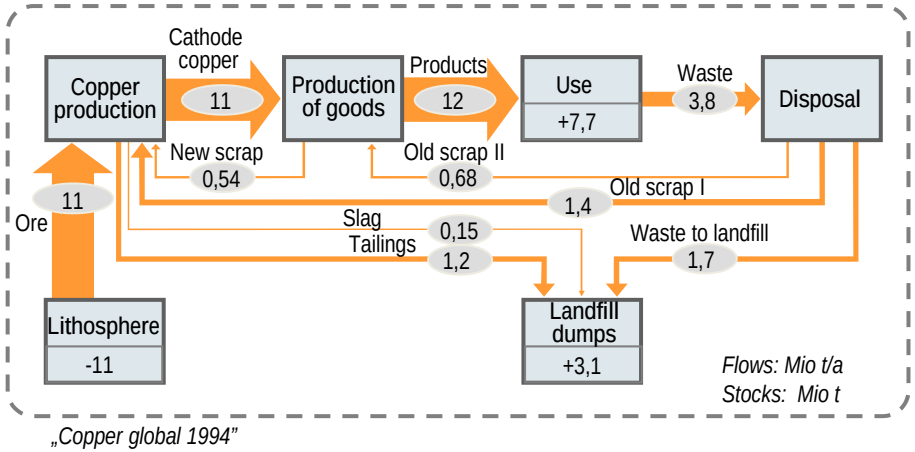
Global copper cycle



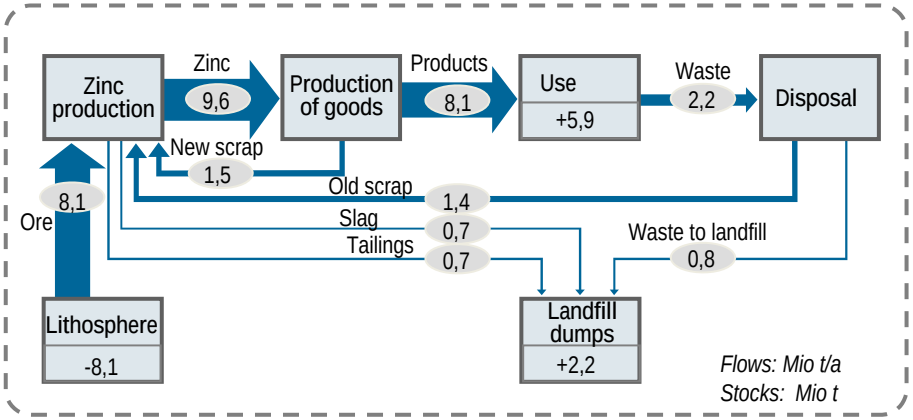
System boundary „zinc global 1996"

Source: Rechberger 2002

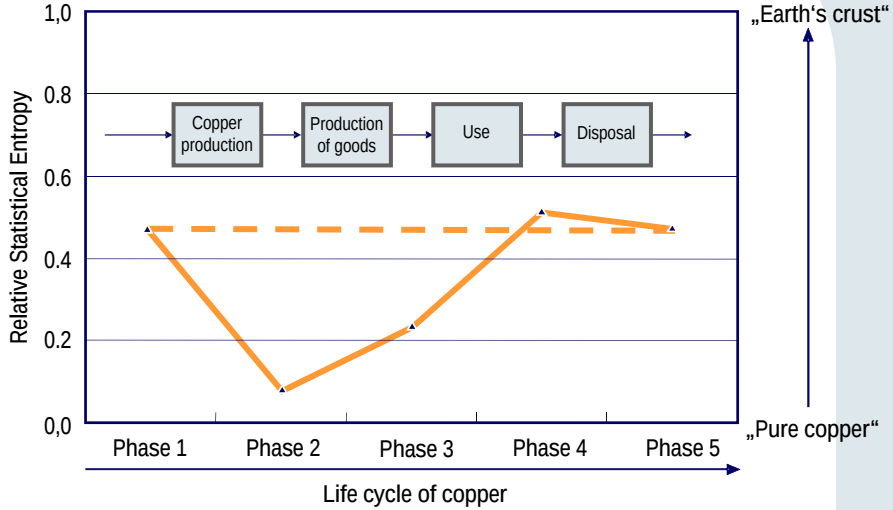
SEA as an indicator for the „performance“ of a system

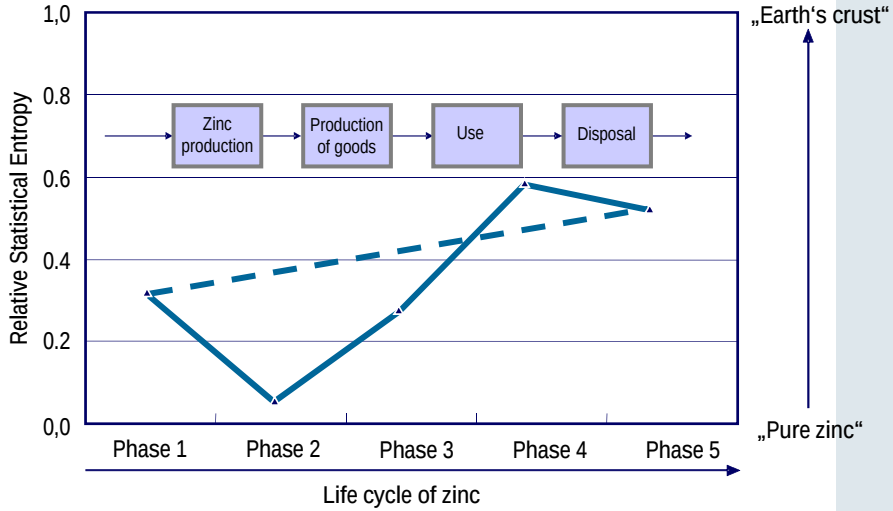


„Copper global 1994“



„Zinc global 1996“





Why is extension required?

Sometimes the chemical speciation is very important, e.g.:

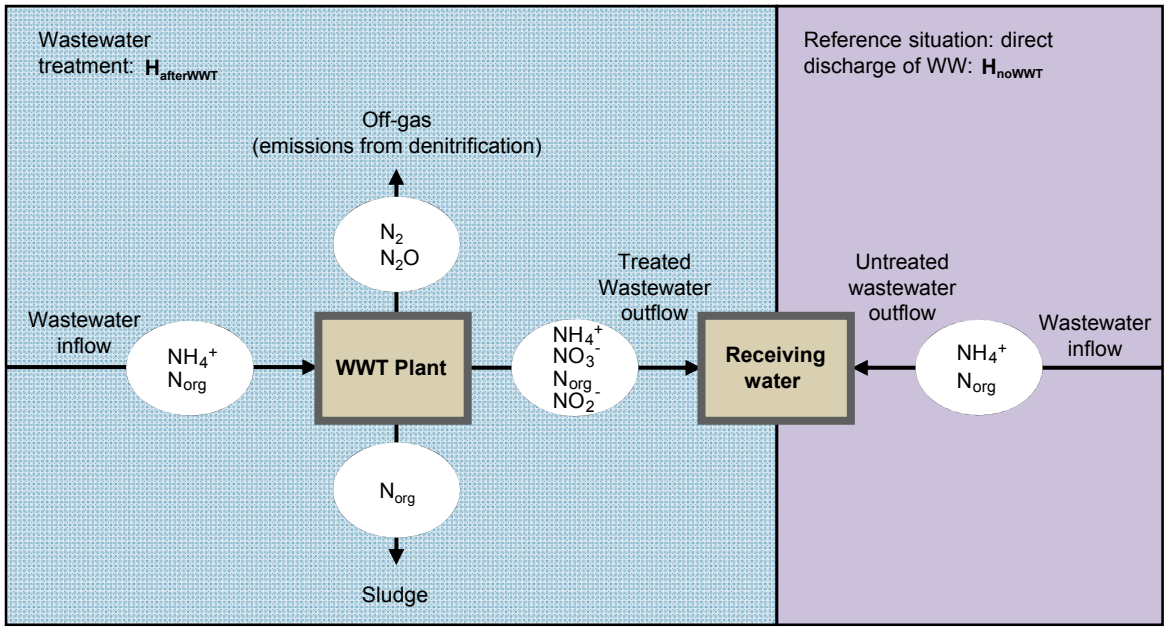
Nitrogen (NO_x, N_2, NH_3,…)

Carbon (CO_2, CO, CH_4, C_xH_y, …)

This requires adaptation of the SEA equations.

Let’s go to the final section: Applications of extended SEA

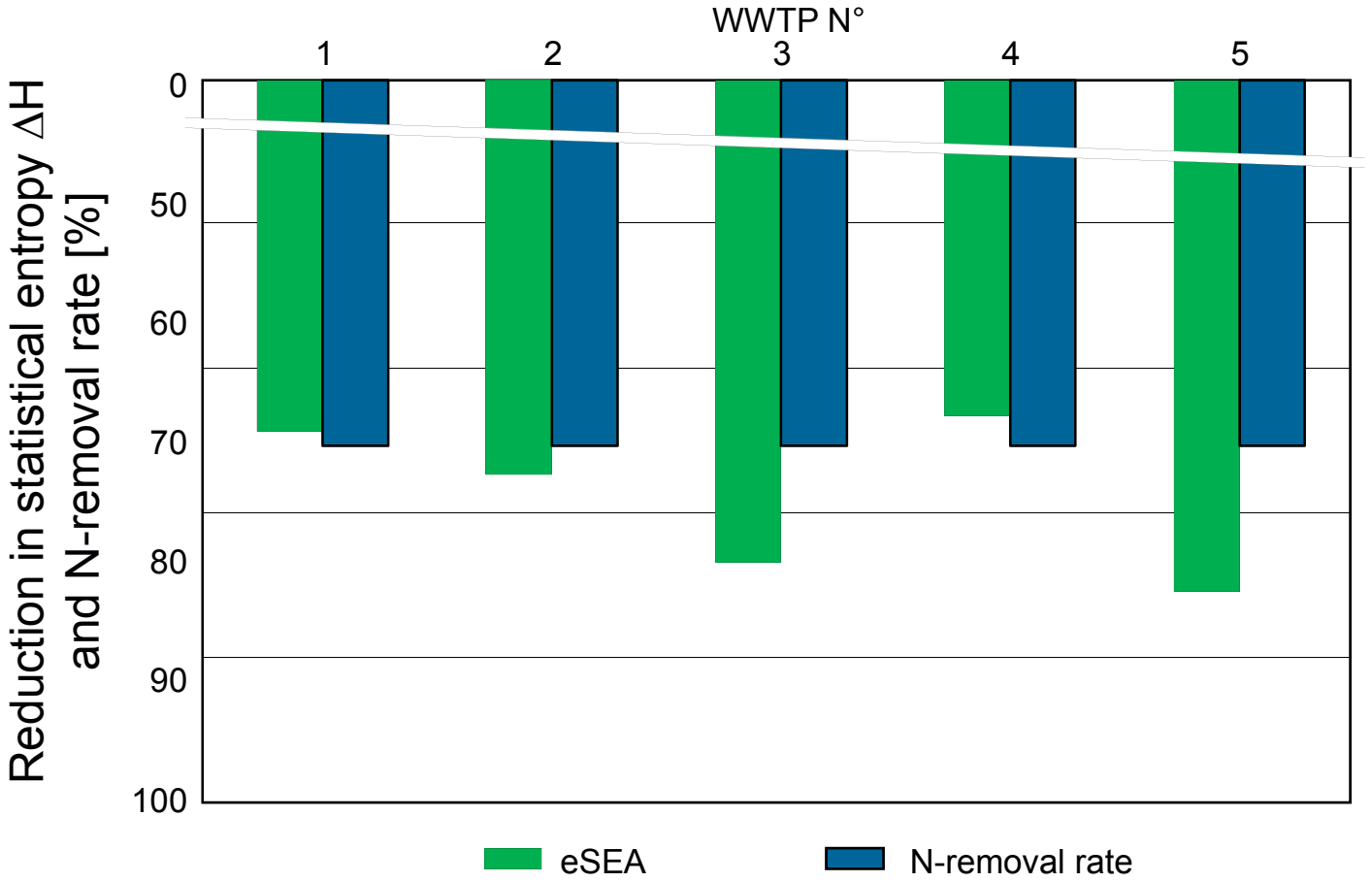
Application to wastewater treatment



Sobańtka & Rechberger, submitted

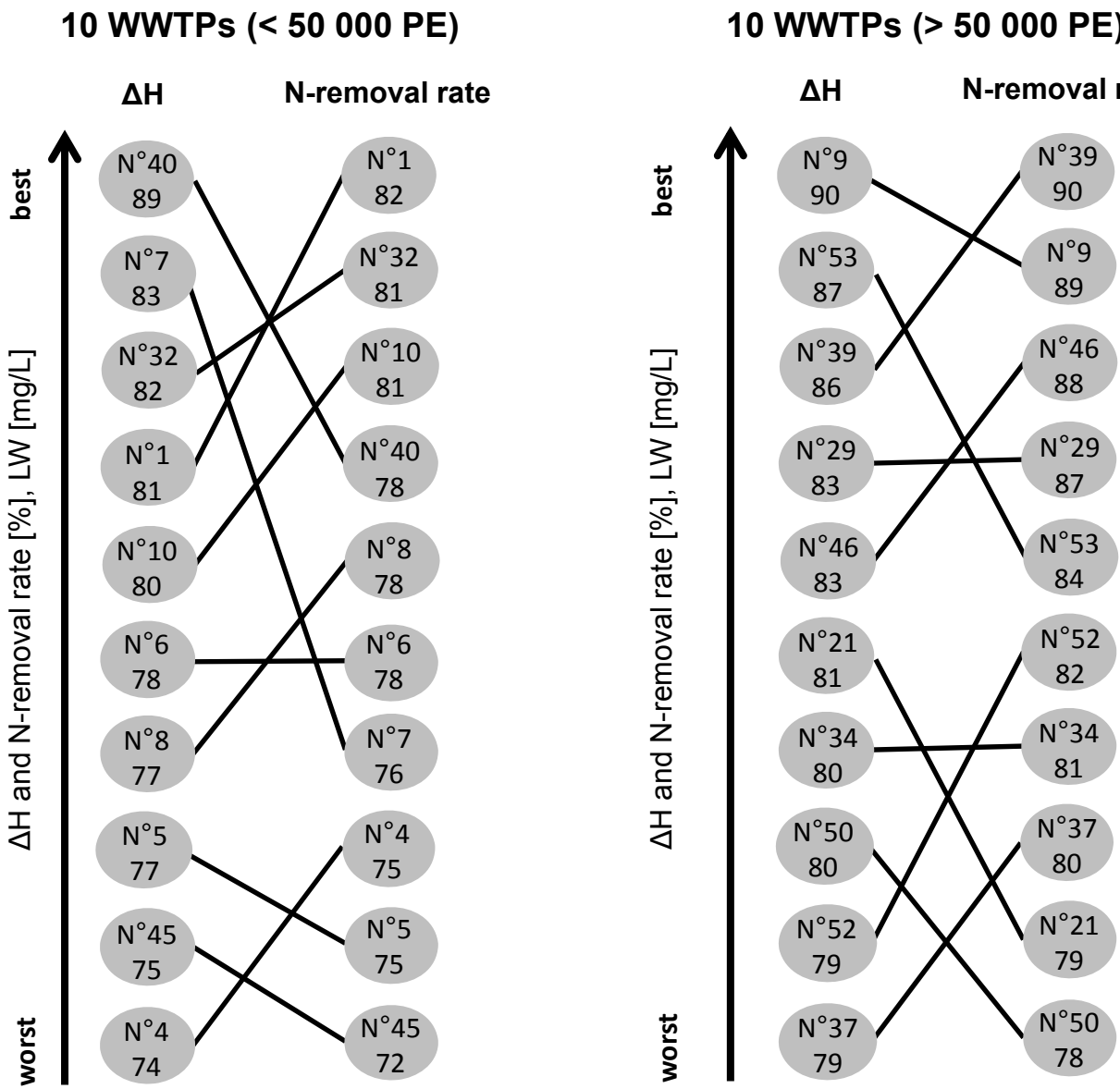
Comparison of 5 WWT facilities

N – removal rate: N_{tot} in the effluent / N_{tot} in the wastewater



Sobańtka & Rechberger, submitted

Ranking of WWT facilities with N-removal rate and ΔH



Comparison of two agricultural regions

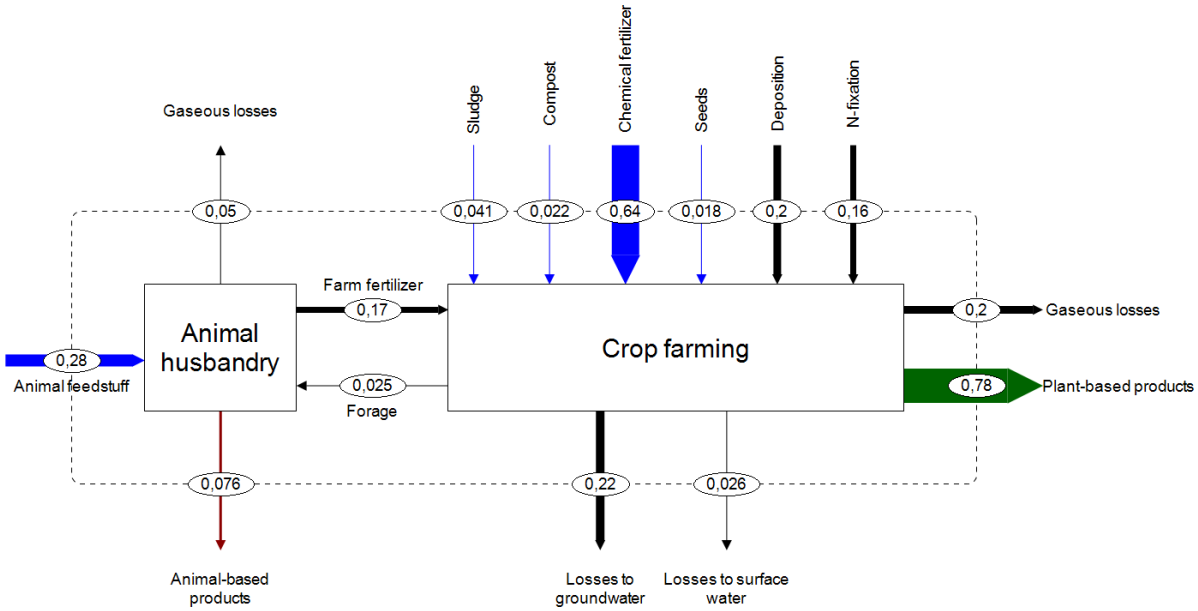


Figure 1: Nitrogen budget Wulka in kgN/ha/a; data related to 1kgN total input

Sobańtka et al., in preparation

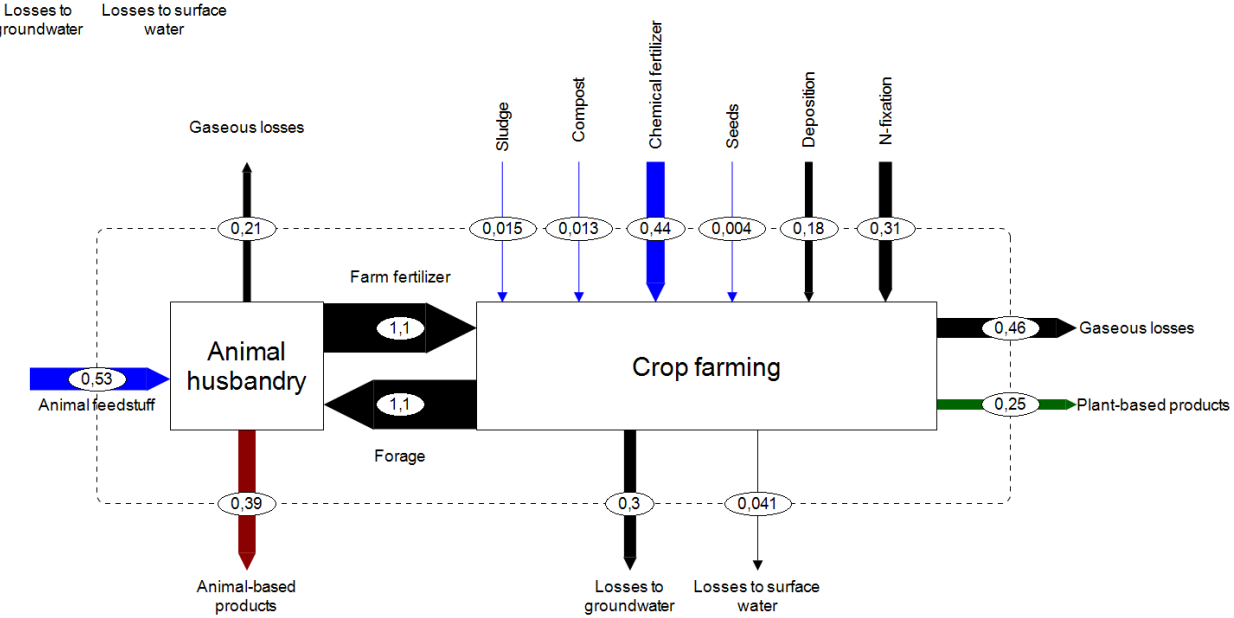
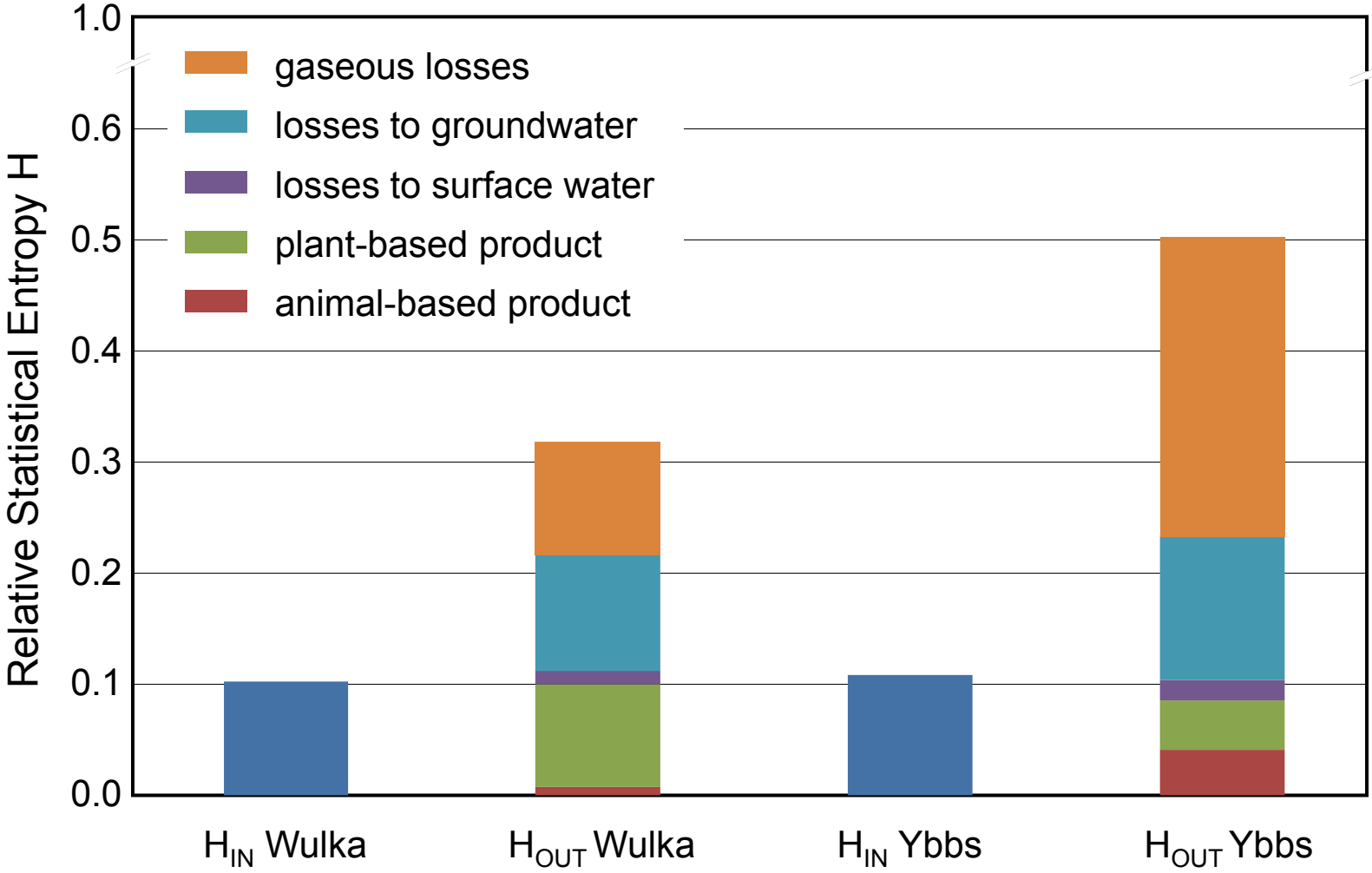


Figure 2: Nitrogen budget Ybbs in kgN/ha/a; data related to 1kgN total input

Comparison of two agricultural regions



Sobańtka et al., in preparation

Publications of SEA

Rechberger, H., Brunner, P.H., A new, entropy based method to support waste and resource management decisions. *Environmental Science and Technology*, **2002**, 34, 4, 809-816.

Rechberger, H., and Graedel, T.E., The European copper cycle: statistical entropy analysis. *Ecological Economics*, **2002**, 42, 1-2, 59-72.

Kaufman, S.; Krishnan, N.; Known, E.; Castaldi, M.; Themelis, N.; Rechberger, H., Examination of the Fate of Carbon in Waste Management Systems through Statistical Entropy and Life Cycle Analysis. *Environmental Science & Technology* , **2008**, 42, 22, 8558-8563.

Yue, Q., Lu, Z.W., Zhi, S.K. Copper cycle in China and its entropy analysis. *Resources, Conservation and Recycling*, **2009**, 53, 12, 680-687.

Sobańtka, A., Rechberger, H., Zessner, M., The extension of Statistical Entropy Analysis to chemical compounds. *Entropy (submitted)*

Sobańtka, A., Rechberger, H., Extended statistical entropy analysis (eSEA) for improving evaluation of Austrian wastewater treatment plants. *Water Science and Technology (submitted)*

Sobańtka, A., Rechberger, H., Pons, M.N., Zessner, M., Re-evaluation of the nitrogen performance in the Benchmarking Simulation Model (BSM). *Water Science and Technology (in preparation)*

Sobańtka, A., Rechberger, H., Zessner, M., Thaler, S., Quantitative comparison of nitrogen budgets in Austrian regions. *Nutrient Cycling in Agroecosystems (in preparation)*